Computational Studies of Gas Transport Properties of Mix Matrix Membrane

AUTHOR(S):

Wu, Chih Yi

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混合マトリクス膜中のガス輸送特性に関する計算機シミュレーション
Computational Studies of Gas Transport Properties of Mix Matrix Membrane

京都大学高等研究院 物質－細胞統合システム拠点　Sivaniah group　Wu Chih Yi

研究成果概要：Membranes used for gas separation has become an important role in industrial application. Mix matrix membranes (MMMs) combines the advantages of polymer and inorganic membranes, that is, adding inorganic fillers into polymer. Fillers with functional groups increases gas selectivity while the polymer acts like a solution of fillers and maintains the membrane structure. Based on our previous work, which we added different functionalized polyhedral oligomeric silsesquioxane (POSS) into polymer of intrinsic microporosity (PIM-1). MMMs with amine and nitro functionalized POSS particles (OAPS and ONPS) results in great dispersibility in PIM-1, enhancement of selectivity in gas separation, and a better aging behavior comparing to PIM-1.
Since characterization of these results in atomic scale may be challenging, Molecular simulation techniques becomes important at microscopic level. Our goal is to simulated OAPS and ONPS MMMs at different weight percentages and studied their mechanical and gas properties.

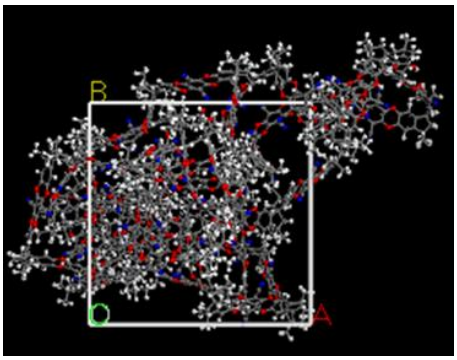

Fig.1 Simulated PIM-1

	Solubility ($\times10^{-3}$ cm^3(STP)/ cm^3 polymer cmHg)	
	This work	Exp
CO_2	1356	700
CH_4	86.1	163
O_2	38.8	39
N_2	34.1	37

Fig.2 PIM-1 simulated solubility with experimental data

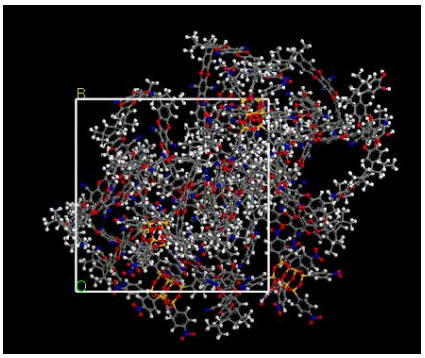

Fig.3 20wt% ONPS MMM

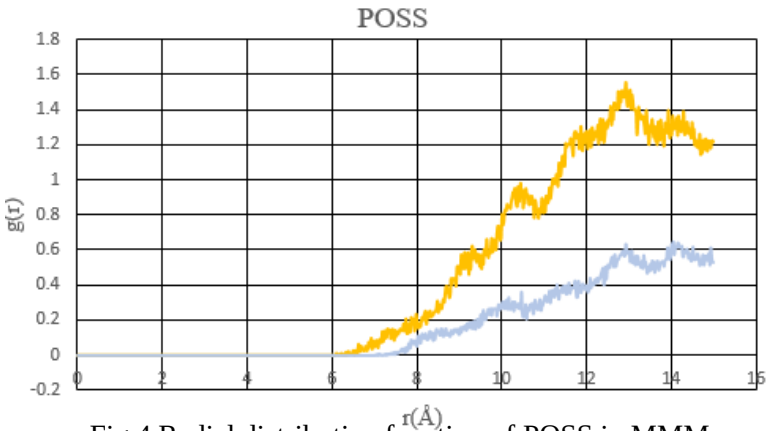

Fig.4 Radial distribution function of POSS in MMMs.
(Yellow: OAPS 20wt%, Gray: ONPS 20wt%)